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The Lagrangian view of energy transfer in turbulent flow

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Abstract. – Hydrodynamic turbulence in 3D is characterized by a non-linear transfer of energy from large to small scales. Here, we provide a geometrical view of energy transfer by relating it to the deformation of fluid volumes under Lagrangian dynamics. The energy flux is parametrized in terms of the coarse-grained velocity difference tensor together with the tensor describing the shape of the volume. Our construction provides an intepretation for the non-trivial time dependence of the energy of relative motion within a "cloud" of Lagrangian particles observed in the direct numerical simulation turbulence.

The non-linear transfer of energy from large to small scales is the hallmark of hydrodynamic turbulence in 3 dimensions. The resulting energy flux is responsible for the dissipation becoming finite in the $\nu \to 0$ limit. Existence of this flux also makes turbulence an intrinsically non-equilibrium phenomenon. The average rate of energy dissipation, or the energy flux ε, plays a key role in Kolmogorov's scaling theory (K41) [1, 2] and is also the subject of one of the few exact results in turbulence theory —the Kolmogorov relation [1, 2]:

$$\frac{\mathrm{d}}{\mathrm{d}x}\langle \Delta u(x)^3 \rangle = -\frac{4}{5}\epsilon + 6\nu \frac{\mathrm{d}^2}{\mathrm{d}x^2}\langle \Delta u(x)^2 \rangle, \tag{1}$$

where $\Delta u(x) \equiv (u(x) - u(0))$. Equation (1) relates the energy flux ε to the $3d$ moment of the structure function in the inertial range (where the effect of the viscosity term on the right-hand side is negligible). Whereas the existence of the *average* energy flux is well established, the fluctuations of the rate of local energy dissipation [2] are understood poorly if at all. Devising a good parametrisation of the *local* energy flux, defined on a given length scale, in terms of the velocity field resolved up to the same scale is essential in the context of large eddy simulations (LES), where the smallest scales of the flow are left unresolved [3, 4]. The LES is arguably the only plausible computational approach to the practical problems of engineering and geophysical turbulence.

Most of the present understanding of the energy flux is based on the Eulerian representation underlying eq. (1). The Lagrangian approach, whereby fluid motion is described in terms of particles advected by the flow, provides a natural framework to describe the dynamical processes underlying the energy transfer [5,6]. The recent progress in the problem of mixing of a passive scalar heavily rests on Lagrangian representation of fluid motion [7,8]. In this letter, we explore the mechanism of energy transfer in Lagrangian terms.

Consider the temporal evolution of the energy of relative motion, $E(t)$, in a cloud of N Lagrangian particles. Assume that at $t = 0$ the cloud particles are randomly distributed over some small volume of characteristic size R_0 in the inertial range. The energy of relative motion at $t = 0$ is estimated on the basis of the Kolmogorov power spectrum, $E(0) \sim \varepsilon^{2/3} R_0^{2/3}$. According to Richardson [9], at long times the characteristic radius of the cloud grows as $\langle R^2(t)\rangle \sim \varepsilon t^3$ so that estimating the relative energy, in the spirit of "mean field" theory, by the characteristic energy on scale $\langle R^2(t)\rangle^{1/2}$, one arrives at $\langle E(t)\rangle \sim \varepsilon t$. On the other hand, the instantaneous time derivative of the relative velocity between two points in the cloud can be determined from the von Karman-Howarth exact relation [10]: $\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}\langle(\boldsymbol{v}(\boldsymbol{x})-\boldsymbol{v}(\boldsymbol{y}))^2\rangle \approx -2\varepsilon$ (provided the separation $|\boldsymbol{x}-\boldsymbol{y}|$ lies in the inertial range of scales). Hence $E(t)$ initially *decreases*, so that the evolution of $E(t)$ is non-monotonic. The initial decrease, due to transfer of energy to smaller scales, is missed by the naive "mean field" argument. Below we shall interpret the crossover between the short- and the long-time behavior of $E(t)$ in terms of the correlation between the "shape" distortion of the Lagrangian cloud and coarse-grained strain. This geometric aspect of Lagrangian evolution is missed in the pure scaling arguments, based only on single scale $R(t)$, but is captured by the proposed parametrization of energy transfer, $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$, in terms of the moment of inertia tensor, $\hat{g}$, of the set of particles, and of the coarse-grained velocity derivative tensor $\hat{M}$. The strain-dependent deformation of the cloud is represented by the $\hat{g}$ tensor, making explicit the geometric aspect of the dynamics. This is the key novelty in our approach.

Consider the evolution of a cloud of N Lagrangian particles, whose location, $(\boldsymbol{x}^1,\ldots,\boldsymbol{x}^N)$, is generated at initial time according to a Gaussian distribution: $P(\boldsymbol{x}^i) = \exp[-((\boldsymbol{x}^i - \boldsymbol{x}^0)^2/2R^2)/(2\pi R^2)^{3/2}]$. The center of mass of the cloud is $\boldsymbol{x}^0$, and its characteristic size is R. The velocity of particle i is denoted $\boldsymbol{v}^i$. The moment of inertia tensor g, characterizing the shape of the cloud [11], the mean velocity, $\boldsymbol{V}$, and the coarse-grained velocity derivative, $\hat{M}$, are defined by

$$g_{ab} \equiv \overline{(x^i-x^0)_a(x^i-x^0)_b}; \qquad \boldsymbol{V} \equiv \overline{\boldsymbol{v}^i}; \qquad M_{ab} \equiv \sum_c g^{-1}_{ac}\overline{(x^i-x^0)_c(v^i-V)_b}, \tag{2}$$

where the overbar denotes the average over a cloud. The coarse-grained velocity gradient tensor, $\hat{M}$, is defined by fitting a linear velocity profile to the set of $\boldsymbol{v}^i$'s. Practically, it is obtained by minimizing $Q = \sum_i\sum_{ab}((v^i-V)_b-(x^i-x^0)_a M_{ab})^2$ with respect to $\hat{M}$. Note that our definition of $\hat{M}$ does not require the knowledge of the derivatives and therefore is accessible experimentally [12–14]. Alternatively, the least-square fitting procedure defines a decomposition of the velocity of particles as

$$v^i_a = V_a + \sum_b (x^i-x^0)_b M_{ba} + u^i_a \tag{3}$$

which explicitly "separates" the center-of-mass motion, the contribution of the coarse-grained velocity gradient and provides a definition of the residual incoherent small-scale component, $\boldsymbol{u}$. The decomposition equation (3) is effectively a scale decomposition: $\boldsymbol{V}$ results from a low-pass filtering, $\boldsymbol{u}$ from a high-pass filtering, and $\sum_b(x^i-x^0)_b M_{ba}$ from a band-pass filtering around $k = 2\pi/R$, analogous in spirit to the one proposed in [11,15]. The kinetic energy, defined as $\mathcal{E} \equiv \frac{1}{2}\overline{\boldsymbol{v}^{i\,2}}$ can be rewritten as $\mathcal{E} = \frac{1}{2}\boldsymbol{V}^2 + E$, where $E = \frac{1}{2}\overline{(\boldsymbol{v}^i-\boldsymbol{V})^2} = \frac{1}{2N^2}\sum_{i<j}(\boldsymbol{v}^i-\boldsymbol{v}^j)^2$. The E-term represents the kinetic energy of relative motion. Using

eq. (3), it can be further decomposed as $E = \frac{1}{2}\,\mathrm{tr}(\hat{g}\hat{M}\hat{M}^\dagger) + \frac{1}{2}\overline{u^{i\,2}}$, thus separating the small-scale coherent and incoherent contributions.

We are interested in the statistical properties of many clouds released in a statistically stationary turbulent flow, maintained by a large-scale forcing, $\boldsymbol{f}$. The ensemble average over many realisations is denoted $\langle\cdots\rangle$. In the statistically steady state, the balance between forcing and viscous dissipation imposes that $\langle \boldsymbol{f}(\boldsymbol{x})\cdot\boldsymbol{v}(\boldsymbol{x})\rangle + \nu\langle\nabla^2\boldsymbol{v}(\boldsymbol{x})\boldsymbol{v}(\boldsymbol{x})\rangle = 0$; the kinetic energy $\mathcal{E}$ of a cloud remains constant: $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E} = 0$. Arguments closely following the von Karman-Howarth original derivation [10] lead to the conclusion that at $t = 0$, $\mathrm{d}\langle E\rangle/\mathrm{d}t < 0$.

By expressing the Lagrangian derivative $\mathrm{d}\langle V^2\rangle/\mathrm{d}t = -\mathrm{d}\langle E\rangle/\mathrm{d}t$ as the sum of the Eulerian derivative, $\partial_t\langle V^2\rangle$, which vanishes in the statistically steady state, and of the contribution originating from the non-linear advection term $\boldsymbol{v}\cdot\nabla\boldsymbol{v}$, and by using the decomposition equation (3), one obtains the relation

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle E\rangle = \langle M_{ab}\sigma_{ab}\rangle, \tag{4}$$

where $\sigma_{ab} = \sum_i (v^i(x)-V)_a(v^i(x)-V)_b$ is the Reynolds stress tensor. Using the decomposition of the velocity field, eq. (3), one finds that $M_{ab}\sigma_{ab} = \mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger) + \sum_{ab} M_{ab}\overline{u_a u_b} \equiv F$. The small-scale contribution to the kinetic energy therefore evolves according to

$$\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}t} = \left\langle\, \mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)\right\rangle + \left\langle \sum_{ab} M_{ab}\overline{u_a u_b}\right\rangle = \langle F\rangle. \tag{5}$$

The transfer term in the RHS of eq. (5) involves correlation of stress and strain decomposed into the sum of the term involving only the coarse-grained velocity derivatives, and the term coupling the coarse-grained strain with the incoherent part of the velocity field. The status of $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$ as an energy transfer term has been explored in several contexts already [3, 4, 16]. The small-scale contribution was accounted for in [16] by an effective renormalisation of $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$. We shall start our analysis by demonstrating that the behavior of the flux F in eq. (5) is controlled by the $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$-term.

We study the evolution of E numerically by following a set of clouds of $N = 2000$ particles. This is done by integrating the Navier-Stokes equations with a pseudospectral, fully resolved code, and by tracking Lagrangian particles with the algorithm introduced in [17]. Several clouds, centered on a 4^3 regular sublattice of the computational box, are injected simultaneously. The size of the clouds was chosen so that the mean separation between particles, initially $\sqrt{3}R$, ranges from dissipative scales ($\sim 4\eta$) to integral scale ($\sim L$). Our conclusions are based on two runs at resolution 96^3 and 192^3, corresponding to $R_\lambda = 65$ and $R_\lambda = 110$.

As expected, the energy of relative motion, E, initially decreases, but after a while starts growing, see fig. 1. The larger the intitial size of the cloud, the later the transition from $\mathrm{d}E/\mathrm{d}t < 0$ to $\mathrm{d}E/\mathrm{d}t > 0$ occurs, at times comparable to the characteristic time scale $\tau(R) \approx \varepsilon^{-1/3}R^{2/3}$ at scale R.

We next examine the energy transfer (eq. (5)), with the goal of parametrizing the $M_{ab}\overline{u_a u_b}$-term, which is in practice one of the central issues in turbulence. One of our main results, illustrated in fig. 2, is the existence of a linear relation between the flux F and $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$. Figure 2 shows the joint pdf of the flux for two values of the size of isotropic clouds, corresponding to an interparticle separation of 8η (fig. 2(a)) and $32\eta \approx 0.4L$ (fig. 2(b)), at $R_\lambda = 110$. The straight line represents the best fit: $F = a\times\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger) + b$. The isoprobability contours are strongly concentrated along these lines, demonstrating a linear dependence between flux, F and $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$. The two quantities are predominantly negative. The coefficients a and b

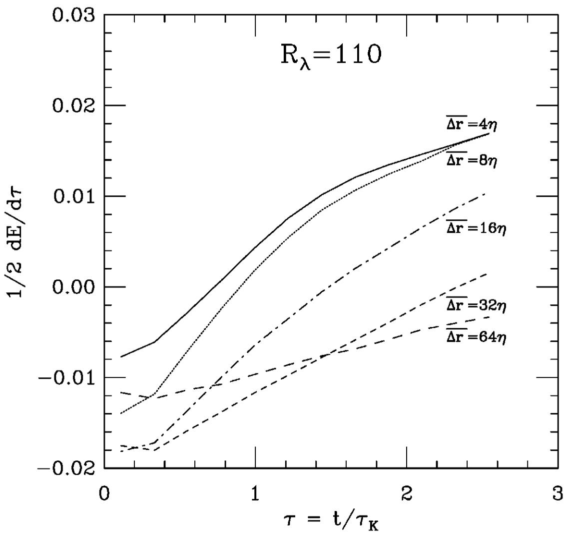

Fig. 1 – The rate of change of E, the energy of the particles in the cloud with respect to the center of mass. As the size of the blob increases, the transition from $\mathrm{d}E/\mathrm{d}t < 0$ to $\mathrm{d}E/\mathrm{d}t > 0$ occurs later. The averages have been constructed from a sample of 270 clouds.

vary with scale, starting from a value $1 \lesssim a$ in the dissipative range, and increase as a function of scale ($a \approx 1.30$ for fig. 2(b)).

The linear relation between F and $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$ allows us to introduce a geometric interpretation of energy transfer. For isotropic clouds ($g_{ab} = R^2\delta_{ab}$), $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger) = R^2(\mathrm{tr}(\hat{S}^3) - \frac{1}{4}\omega \cdot \hat{S} \cdot \omega)$, where $\hat{S} = \frac{1}{2}(\hat{M} + \hat{M}^\dagger)$ is the strain, and ω is the vorticity. The density of F, defined as the product of F by the joint probability distribution function of $\mathrm{tr}(\hat{S}^3)$ and $\omega \cdot \hat{S} \cdot \omega$, is shown in fig. 3. The iso-density lines are concentrated around the line $\frac{1}{4}\omega \cdot \hat{S} \cdot \omega = 0$, demonstrating that $\mathrm{tr}(\hat{S}^3)$ is the dominant term for energy transfer. Neglecting the vortex stretching term, the sign of F is related to the properties of the eigenvalues of the strain, $\hat{S}$. Indeed, denoting the eigenvalues of $\hat{S}$ by $\lambda_1 \geq \lambda_2 \geq \lambda_3$ (with $\lambda_1 + \lambda_2 + \lambda_3 = 0$ due to incompressibility, so $\lambda_1 > 0$ and $\lambda_3 < 0$), $\mathrm{tr}(\hat{S}^3) = \lambda_1^3 + \lambda_2^3 + \lambda_3^3 = 3\lambda_1\lambda_2\lambda_3$, so $-\mathrm{tr}(\hat{S}^3)$ has the sign of λ_2. This sign is well documented to be predominantly positive at the level of the velocity derivative at one point [18] and for the coarse-grained velocity derivative [16]. This property explains the initial sign of $\mathrm{d}E/\mathrm{d}t$. Alternatively, since the negative sign of $\mathrm{d}E/\mathrm{d}t$ follows from the von Karman-Howarth argument [10], the latter can be held as a proof that the energy flux is dominated by strain "sheets", *i.e.* $\lambda_2 > 0$, configurations.

The coarse-grained strain, $\hat{S}$ also determines the shape deformation of the cloud. Indeed, the evolution of the shape is governed by $\mathrm{d}\hat{g}/\mathrm{d}t = (\hat{g} \cdot \hat{M} + \hat{M}^\dagger \cdot \hat{g})$. This may be reduced, by rotating the coordinates by $\hat{R}(t)$ ($\hat{g} \to \hat{R}(t)\underline{\hat{g}}\hat{R}(t)^\dagger$, $\hat{M} \to \hat{R}(t)\underline{\hat{M}}\hat{R}(t)^\dagger$), so as to follow vorticity ($\hat{R}(t)^\dagger \frac{\mathrm{d}}{\mathrm{d}t}\hat{R}(t) = -\hat{\Omega}$, where $\Omega = \frac{1}{2}(\hat{M} - \hat{M}^\dagger)$, to $\frac{\mathrm{d}\underline{\hat{g}}}{\mathrm{d}t} = (\underline{\hat{g}} \cdot \underline{\hat{S}} + \underline{\hat{S}} \cdot \underline{\hat{g}})$, where $\underline{\hat{S}} = (\underline{\hat{M}} + \underline{\hat{M}}^\dagger)/2$. This implies that the cloud is stretched (compressed) in the direction corresponding to positive (negative) eigenvalues of $\underline{\hat{S}}$. Consequently, the principal axis of the $\hat{g}$ tensor along the fast stretching direction of $\hat{S}$ becomes much larger than that along the compressing direction(s). The nearly singular $\hat{g}$ tensor will project out the contribution of compressive strain eigenvalue to the trace $\mathrm{tr}(\hat{g}\hat{S}^3) = \mathrm{tr}(\underline{\hat{g}}\underline{\hat{S}}^3)$. As a result $\mathrm{tr}(\hat{g}\hat{S}^3)$ will become positive.

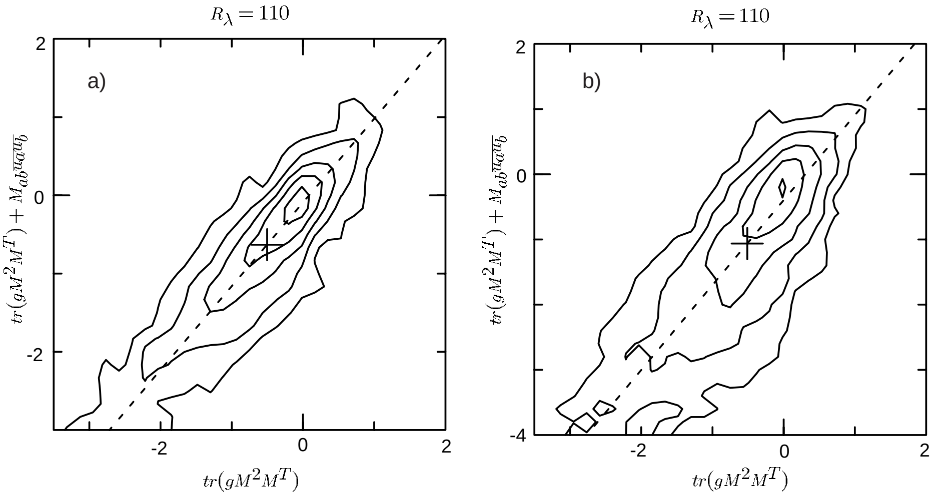

Fig. 2 – Joint probability distribution functions of $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$ and the flux $F = \mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger) + \sum_{ab} \overline{u_a u_b}$ for two values of the mean interparticle separation: 8η (a) and $32\eta \approx 0.4L$ (b). The histograms have been constructed with 4096 clouds. The two quantities have been normalized by the rms of $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$. The isoprobability contours are logarithmically spaced, and separated by a factor $\sqrt{10}$. The isocontours follow closely the best fit line, $F = a \times \mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger) + b$, demonstrating the quality of the parametrisation of the flux by $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$. All quantities are made dimensionless by dividing by $\sqrt{\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^T)^2}$. The mean value of $(\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger), F)$ is indicated by a cross.

Since it is the dominant term in $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$, the flux changes sign, as observed numerically. Thus the crossover from negative to positive $\mathrm{d}E/\mathrm{d}t$ is due to the development of a correlation between the shape of the cloud and the strain. It is exactly this correlation or alignment of all interparticle vectors with the fast stretching direction which distinguishes the initial cloud from the Lagrangian cloud at $t > 0$.

We mention that the numerical results and the qualitative picture discussed here are consistent with the prediction of the stochastic model of [16]. In the model, we computed directly the flux $\langle \mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^T)\rangle$ by a Monte Carlo algorithm. The initially negative value of the flux becomes positive during the evolution as the cloud distorts. The result is independent of the precise value of the parameters chosen to model the effects of smaller scales.

These considerations lead to an intuitively appealing geometric picture of the energy flux: energy transfer to smaller scales is related to the deformation of the overall shape, which, because of the predominance of sheet-like strain configurations ($\lambda_2 < 0$), is dominated by compression. Our numerical results indicate that the change of sign of $\mathrm{d}E/\mathrm{d}t$ occurs well before the shape of the cloud develops the folding, observed in mixing experiments [5]. At very long times, a non-trivial distribution of the shape of the cloud is observed [11].

The argument we have used for velocity applies as well in the case of a passive scalar, θ. A decomposition analogous to eq. (3) can be used for the scalar:

$$\theta^i = \Theta + \sum_a (x^i - x^0)_a G_a + \phi^i, \tag{6}$$

where Θ is the mean value of the scalar, G the coarse gradient, obtained by fitting a linear function to the values of θ^i, and ϕ the incoherent part of the scalar. The expression for the scalar flux, analogous to eq. (5) is $\langle F_\theta \rangle = \langle \sum_{abc} g_{ab} M_{bc} G_c G_a \rangle + \langle G_a \overline{u_a \phi} \rangle$. The von

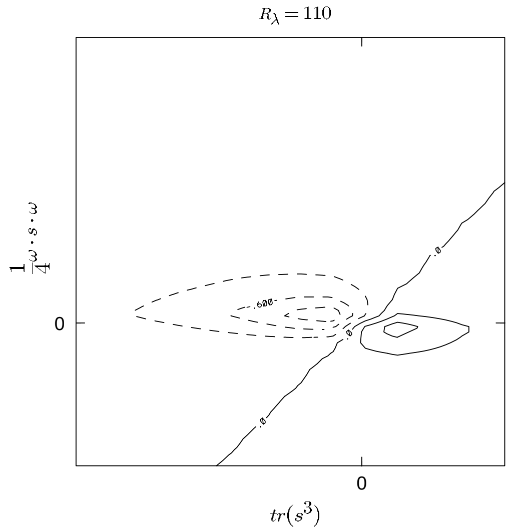

Fig. 3 – Isodensity contours of $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^\dagger)$ as a function of the strain skewness $\mathrm{tr}(\hat{S}^3)$ (horizontal) and the vortex stretching $1/4\omega \cdot \hat{S} \cdot \omega$ for isotropic clouds, and for an interparticle spacing of $32\eta \approx 0.4L$. All quantities are made dimensionless by dividing by $\mathrm{tr}(\hat{S}^2)^{3/2}$. The contours are strongly aligned with the zero-stretching line, demonstrating that most of the flux comes from strain skewness.

Karman-Howarth argument can be easily generalized to the passive scalar case, and leads to the conclusion that the small-scale scalar energy, $E_\theta \equiv \frac{1}{2}\sum_i(\theta_i - \Theta)^2$ initially decreases: $\mathrm{d}E_\theta/\mathrm{d}t < 0$ at $t = 0$. At later times, as particles are drifting away from each other, E_θ grows. Numerically, we found that the incoherent term of the scalar energy flux is highly correlated with the coarse-grained quantity, as was the case for velocity. This fact enables us to interpret the non-monotonic dependence of the small-scale passive scalar energy. Indeed, the passive scalar gradient is known to align with the most contracting direction of the rate of strain tensor [18]. As a consequence, for an intially isotropic cloud of particles ($g_{ab} = R^2\delta_{ab}$), the sign of $\langle\sum_{abc} g_{ab}M_{bc}G_cG_a\rangle = \langle R^2\sum_{bc} S_{bc}G_bG_c\rangle$ is initially negative. As the cloud evolves, the contraction induced by the most compressing eigenvalue of the rate of strain tensor reduces the corresponding component of g, thus diminishing the negative contribution to the flux, and eventually changing the sign of the scalar energy transfer.

Our discussion so far has been restricted to the 3-dimensional case. We observe that the energy flux based on $\mathrm{tr}(\hat{g}\hat{M}^2\hat{M}^T)$ is identically zero in 2 dimensions. This is consistent with the fact that turbulence in 2 dimensions is characterized by an energy flux to *large scales*, hence an inverse energy cascade.

In conclusion, we have shown how to parametrize the energy flux in terms of the coarse-grained velocity gradient and the shape tensor defined on a cloud of Lagrangian particles and provided a geometric interpretation of the observed non-monotonic behavior of the energy of relative Lagrangian motion. Similar non-monotonic behavior is observed for the evolution of turbulent kinetic energy in homogeneous shear flow [19]. These results are relevant both for fundamental understanding and for modelling of turbulent flows.

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